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NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	DEC 01	ChemPort single article sales feature unavailable
NEWS 3	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 4	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 5	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS 6	FEB 10	COMPENDEX reloaded and enhanced
NEWS 7	FEB 11	WTEXTILES reloaded and enhanced
NEWS 8	FEB 19	New patent-examiner citations in 300,000 CA/CAplus patent records provide insights into related prior art
NEWS 9	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS 10	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS 11	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS 12	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS 13	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS 14	FEB 25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS 15	MAR 06	INPADOCDB and INPAFAMDB enhanced with new display formats
NEWS 16	MAR 11	EPFULL backfile enhanced with additional full-text applications and grants
NEWS 17	MAR 11	ESBIOBASE reloaded and enhanced
NEWS 18	MAR 20	CAS databases on STN enhanced with new super role for nanomaterial substances
NEWS 19	MAR 23	CA/CAplus enhanced with more than 250,000 patent equivalents from China
NEWS 20	MAR 30	IMSPATENTS reloaded and enhanced
NEWS 21	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS 22	APR 07	STN is raising the limits on saved answers
NEWS 23	APR 24	CA/CAplus now has more comprehensive patent assignee information
NEWS 24	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS 25	APR 28	CAS patent authority coverage expanded
NEWS 26	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 27	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS 28	MAY 08	STN Express, Version 8.4, now available
NEWS 29	MAY 11	STN on the Web enhanced

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 NEWS 30  MAY 11  BEILSTEIN substance information now available on
                  STN Easy
 NEWS 31  MAY 14  DGENE, PCTGEN and USGENE enhanced with increased
                  limits for exact sequence match searches and
                  introduction of free HIT display format
 NEWS 32  MAY 15  INPADOCDB and INPAFAMDB enhanced with Chinese legal
                  status data

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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FILE 'HOME' ENTERED AT 10:49:55 ON 20 MAY 2009

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DICTIONARY FILE UPDATES:  18 MAY 2009  HIGHEST RN 1147182-17-9

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=>
Uploading C:\Program Files\Stnexp\Queries\10538196genC.str
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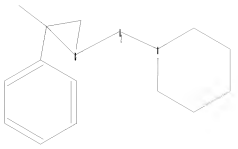

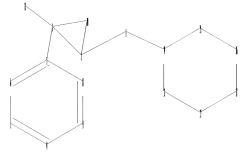

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ring nodes :
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ring bonds :
2-3  2-10  3-10  4-5  4-9  5-6  6-7  7-8  8-9  12-13  12-17  13-14  14-15  15-16
16-17
exact/norm bonds :
2-3  2-10  3-10  12-13  12-17  13-14  14-15  15-16  16-17
exact bonds :
1-2  1-14  3-7  3-11
normalized bonds :
4-5  4-9  5-6  6-7  7-8  8-9


Match level :
1:CLASS  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:CLASS  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
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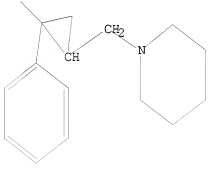


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Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss full
FULL SEARCH INITIATED 10:50:59 FILE 'REGISTRY'
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FULL SCREEN SEARCH COMPLETED - 2622 TO ITERATE

100.0% PROCESSED 2622 ITERATIONS 346 ANSWERS
SEARCH TIME: 00.00.01

L2 346 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
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FILE COVERS 1907 - 20 May 2009 VOL 150 ISS 21
FILE LAST UPDATED: 19 May 2009 (20090519/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate

=> s l2
L3 22 L2

=> s l3 and pd<20030500
23788219 PD<20030500
(PD<20030500)
L4 15 L3 AND PD<20030500

=> d l4 1-15 abs ibib hitstr

L4 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
AB In this study, using the new sigma1/2 (σ1/2) compound MR200, its parent drug haloperidol and the σ ligand 1,3-di-o-tolylguanidine (DTG), the authors have investigated the role of striatal σ receptors in the control of basal dopamine (DA) outflow, by coupling in vitro binding expts. and in vivo microdialysis in the striatum of halothane-anesthetized rats. MR200 with respect to haloperidol, exhibits high affinity for σ1 (1.5 nM) and σ2 (21.9 nM) receptors, but only negligible affinity for DA receptors. Compared to DTG, MR200 has similar selectivity across neurotransmitter systems, and 46 times higher

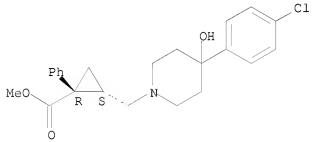
affinity for σ1 receptors. Intrastriatal application of MR200 at 10, but not 0.1 or 1 μM, elicited a pronounced decrease in striatal DA release (−45% of control values). This inhibitory effect was preceded by a transient increase in DA release (+50% over baseline) after 100 μM MR200 administration. DTG at 100, but not 10 μM, significantly reduced DA release (−40%). Haloperidol, while increasing DA release at 1 μM, induced a delayed decrease in DA release after 10 μM application. Finally, haloperidol (10 μM) did not modify the inhibitory effect of 10 μM MR200. These results show that striatal σ receptors control striatal DA release in resting conditions.

ACCESSION NUMBER: 2003:828834 CAPLUS
DOCUMENT NUMBER: 140:157786
TITLE: Intrastriatal administration of sigma ligands inhibits basal dopamine release in vivo
AUTHOR(S): Moison, Delphine; De Deurwaerdere, Philippe; Cagnotto, Alfredo; Marrazzo, Agostino; Prezzavento, Orazio; Ronsisvalle, Giuseppe; Mennini, Tiziana; Spampinato, Umberto
CORPORATE SOURCE: Unite Mixte de Recherche-Centre National de la Recherche Scientifique, Laboratoire de Neuropsychobiologie des Desadaptations, Universite Victor Segalen Bordeaux 2, Bordeaux, 5541, Fr.
SOURCE: Neuropharmacology (2003), 45(7), 945-953
CODEN: NEPHBW; ISSN: 0028-3908
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 654641-67-5, MR 200 oxalate
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(intrastriatal administration of sigma ligands inhibits basal dopamine release in vivo in rats)
RN 654641-67-5 CAPLUS
CN Cyclopropanecarboxylic acid, 2-[[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]methyl]-1-phenyl-, methyl ester, (1R,2S)-rel-(+)-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

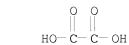
CRN 403789-28-6
CMF C23 H26 Cl N O3

Rotation (+). Absolute stereochemistry unknown.



CM 2

CRN 144-62-7
CMF C2 H2 O4



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

AB A three-dimensional mol. model of the transmembrane domain of the κ-opioid receptor in a phospholipid bilayer is presented. The endogenous ligand, dynorphin A (1), and synthetic ligands, benzomorphan-based compds. (2a, 2b), are docked into the model. We report the results of a 500 ps mol. dynamics simulation of these protein-ligand complexes in a simplified bilayer of 97 mols. of the lipid dipalmitoylphosphatidylcholine and 26 water mols. per lipid. The simulations explore the stability and conformational dynamics of the model in a phospholipid bilayer; we also investigate the interactions of the protein with its ligands. Mol. simulation of the receptor-ligand complexes, endogenous and synthetic, has confirmed the existence of different binding domains for peptide and non-peptide ligands. Similarities are found in the dynamics and binding mode of all conformations of the synthetic ligands studied. The protonated hydrogen of the benzomorphan is always involved in an H-bond with Asp138, and other potentially stabilizing receptor-ligand interactions found involve the hydroxyl substituent on the benzomorphan, which may form an H-bond with Tyr139 or Gly190 according to the different mols. The ester group of 2a may therefore form an H-bond with Ile316, while the carbonyl group of 2b forms an H-bond with Gln115 and Tyr312. The remaining part of the ligand is located in the extracellular portion of the pocket. It is surrounded by hydrophobic residues in the transmembrane region (TM), and it interacts with different sets of residues. The results obtained are in general agreement with site-directed mutagenesis data that have highlighted the importance of all TM regions for synthetic-ligand affinity with the κ-opioid receptor.

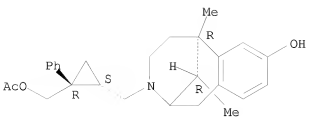
ACCESSION NUMBER: 2002:737864 CAPLUS
DOCUMENT NUMBER: 137:381449
TITLE: κ-Opioid Receptor Model in a Phospholipid Bilayer: Molecular Dynamics Simulation
AUTHOR(S): Iadanza, Manuela; Hoeltje, Monika; Ronsisvalle, Giuseppe; Hoeltje, Hans-Dieter
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Catania, Catania, 95125, Italy
SOURCE: Journal of Medicinal Chemistry (2002), 45(22), 4838-4846
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT 476337-34-5 476337-35-6
RL: BSU (Biological study, unclassified); BIOL (Biological study) (ligand, docking; mol. dynamics simulation of a κ-opioid receptor model in a phospholipid bilayer)

RN 476337-34-5 CAPLUS

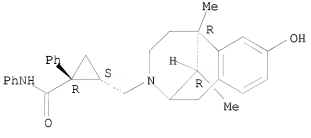
CN 2,6-Methano-3-benzazocin-8-ol, 3-[[(1R,2S)-2-[(acetyloxy)methyl]-2-phenylcyclopropyl]methyl]-1,2,3,4,5,6-hexahydro-6,11-dimethyl-, (6R,11R)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 476337-35-6 CAPLUS
CN Cyclopropanecarboxamide, N,1-diphenyl-2-[[(6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

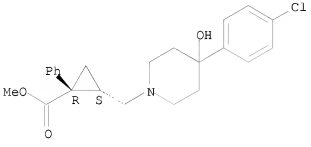
AB New racemic and chiral Me 2-{[4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl]methyl}-1-phenylcyclopropanecarboxylate derivs. were synthesized in order to obtain sigma ligands with increased affinity and selectivity compared to (+)-MPCB and haloperidol. The cis-(+)-7 racemic mixture showed a better binding affinity and selectivity than the (±)-8 trans isomers. Between the two cis enantiomers, (+)-7, with configuration (IR,2S), showed a very high affinity and the best selectivity for σ1. All compds. synthesized (7-9) showed a reduced or negligible affinity for opioid and dopaminergic D1 and D2 receptors. Nociceptive in vivo test confirms that (+±)-7 (namely MR200), such as non-selective antagonist haloperidol. increased the analgesic effect induced by the Kt opioid selective ligand U50,4881I and reversed the inhibiting effect of (+)-pentazocine on analgesia.

ACCESSION NUMBER: 2001:915611 CAPLUS
DOCUMENT NUMBER: 136:241509
TITLE: Opioid and sigma receptor studies. New developments in the design of selective sigma ligands
AUTHOR(S): Ronsisvalle, Giuseppe; Marrazzo, Agostino; Prezzavento, Orazio; Cagnotto, Alfredo; Mennini, Tiziana; Parenti, Carmela; Scoto, Giovanna M.
CORPORATE SOURCE: IUPAC Commission, Department of Pharmaceutical Sciences, University of Catania, Catania, 95125, Italy
SOURCE: Pure and Applied Chemistry (2001), 73(9), 1499-1509
CODEN: PACHAS; ISSN: 0033-4545
PUBLISHER: International Union of Pure and Applied Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 403789-27-5P 403789-28-6P 403789-29-7P

403789-30-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of σ-ligands with increased affinity and selectivity)

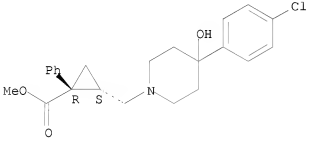
RN 403789-27-5 CAPLUS
CN Cyclopropanecarboxylic acid, 2-[[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]methyl]-1-phenyl-, methyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



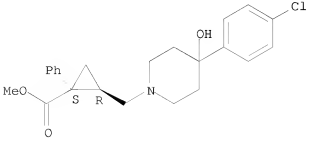
RN 403789-28-6 CAPLUS
CN Cyclopropanecarboxylic acid, 2-[[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]methyl]-1-phenyl-, methyl ester, (1R,2S)-rel-(+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



RN 403789-29-7 CAPLUS
CN Cyclopropanecarboxylic acid, 2-[[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]methyl]-1-phenyl-, methyl ester, (1S,2R)-rel-(-)- (CA INDEX NAME)

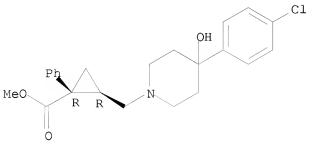
Rotation (-). Absolute stereochemistry unknown.



RN 403789-30-0 CAPLUS

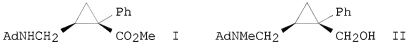
CN Cyclopropanecarboxylic acid, 2-[[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]methyl]-1-phenyl-, methyl ester, (1R,2R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
GI



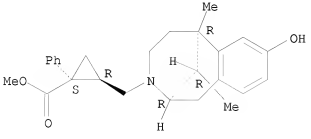
AB In a previous study we found that substitutions of the (+)-cis-N-normetazocine nucleus of (+)-MPCB with 1-adamantanamine provide the compound (±)-I (Ad = 1-adamantyl) with high affinity and selectivity for σ receptors. Starting with this result, we have synthesized a new series of eight 1-phenyl-2-cyclopropylmethylamines structurally related to (±)-I (Ad = 1-adamantyl), and binding affinities with respect to σ1, σ2, opioid and dopaminergic D2 receptors have been reported. All compds. showed a negligible opioid and dopaminergic affinity and high selectivity for σ receptors. Modifications of the amino moiety and COOMe group of I provide compds. with different σ1 and σ2 binding affinity and selectivity. Moreover, we have also synthesized the resp. enantiomers of compds. (±)-I and (±)-II in order to evaluate the enantioselectivity for σ1 and σ2 receptors. The binding data showed that COOMe on the cyclopropane ring was more critical for enantioselectivity than the hydroxymethylenic group. In fact, the (-)-I enantiomer showed a preference for σ1 whereas (+)-I showed a preference for σ2.

ACCESSION NUMBER: 2001:516914 CAPLUS
DOCUMENT NUMBER: 135:288534
TITLE: Synthesis and pharmacological evaluation of potent and enantioselective σ1 and σ2 ligands
AUTHOR(S): Marrazzo, Agostino; Prezzavento, Orazio; Pasquinucci, Lorella; Vittorio, Franco; Ronsisvalle, Giuseppe
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Catania, Catania, 95125, Italy
SOURCE: Farmaco (2001), 56(3), 181-189
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:288534
IT 149343-50-0 199999-64-9 199999-67-2

199999-69-4 199999-71-8 364324-46-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation and pharmacol. evaluation of potent and enantioselective σ1 and σ2 ligands)

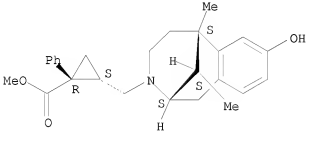
RN 149343-50-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



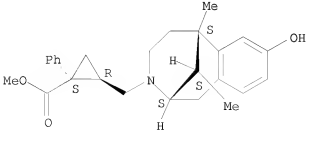
RN 199999-64-9 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 199999-67-2 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1S,2R)- (CA INDEX NAME)

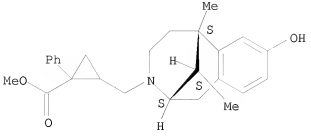
Absolute stereochemistry. Rotation (+).



RN 199999-69-4 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl

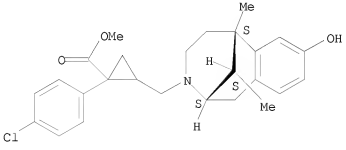
ester (CA INDEX NAME)

Absolute stereochemistry.



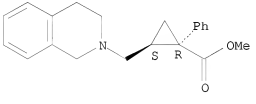
RN 199999-71-8 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(4-chlorophenyl)-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 364324-46-9 CAPLUS
CN Cyclopropanecarboxylic acid, 2-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]-1-phenyl-, methyl ester, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
AB Two novel series of κ opioid receptor agonist analogs of MPCB-GRRI and MPCB-RRI, hybrid ligands of MPCB ((-)-cis-N-(2-phenyl-2-carbomethoxy)cyclopropylmethyl-N-normetazocine) and of the C-terminal fragments of dynorphin A(1-8), have been synthesized. The critical functional groups of the peptide fragments of hybrid compds. were maintained, and the binding affinities and selectivities for compds. 1-40 to μ, δ, and κ opioid receptors were analyzed. Compds. 15 and 16, MPCB-Gly-Leu-NH-(CH2)n-NH-C(:NH)-C4H9 (n = 5, 6), displayed high affinity and selectivity for κ opioid receptors

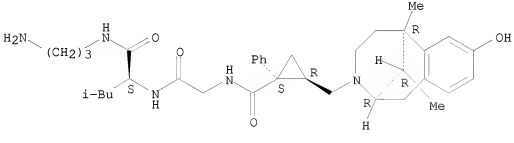
(Kiκ = 6.7 and 5.3 nM, Kiμ/Kiκ = 375 and 408, and Kiδ/Kiκ = 408 and 424, resp.). Since κ agonists may also cause psychotomimetic effects by interaction with σ sites, binding assays to σ1 sites were performed where compds. 15 and 16 showed negligible affinity (Ki > 10 000). Compds. 15 and 16 were further characterized in vivo and showed potent antinociceptive activity in mouse abdominal constriction tests (ED50 = 0.88 and 1.1 mg/kg, resp.), fully prevented by nor-BNI. Thus, these novel analogs open an exciting avenue for the design of peptidomimetics of dynorphin A(1-8).

ACCESSION NUMBER: 2000:490061 CAPLUS
DOCUMENT NUMBER: 133:252708
TITLE: Nonpeptide Analogues of Dynorphin A(1-8): Design, Synthesis, and Pharmacological Evaluation of κ-Selective Agonists
AUTHOR(S): Ronsisvalle, Giuseppe; Pasquinucci, Lorella; Pittala, Valeria; Marrazzo, Agostino; Prezzavento, Orazio; Di Toro, Rosanna; Falcucci, Barbara; Spampinato, Santi
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Catania, Catania, 95125, Italy
SOURCE: Journal of Medicinal Chemistry (2000), 43(16), 2992-3004
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:252708

IT 294624-70-7P 294624-71-8P 294624-72-9P
294624-73-0P 294624-90-1P 294624-91-2P
294624-92-3P 294624-93-4P 294625-27-7P
294625-28-8P 294625-29-9P 294625-30-2P
294625-31-3P 294625-32-4P 294625-33-5P
294625-34-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and binding affinity of κ-selective agonists)

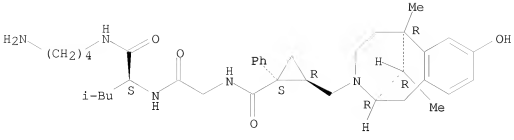
RN 294624-70-7 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-(3-aminopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



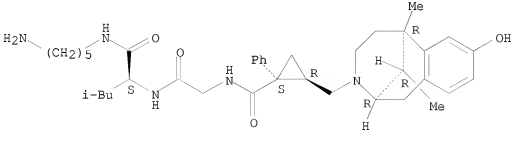
RN 294624-71-8 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-(4-aminobutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 294624-72-9 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-(5-aminopentyl)- (9CI) (CA INDEX NAME)

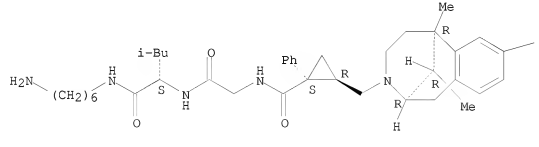
Absolute stereochemistry.



RN 294624-73-0 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-(6-aminohexyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



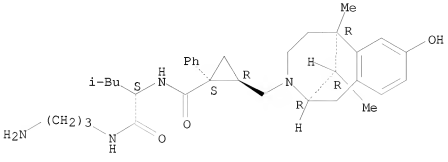
PAGE 1-B

OH

RN 294624-90-1 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[(3-aminopropyl)amino]carbonyl]-3-

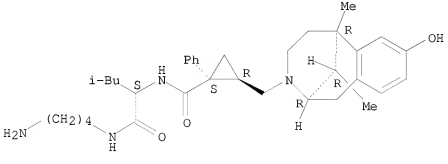
methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



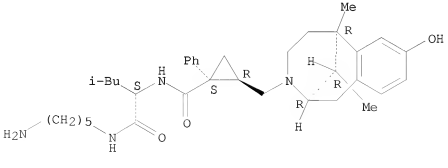
RN 294624-91-2 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[(4-aminobutyl)amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 294624-92-3 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[(5-aminopentyl)amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

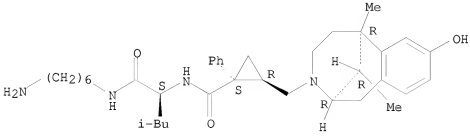
Absolute stereochemistry.



RN 294624-93-4 CAPLUS

CN Cyclopropanecarboxamide, N-[(1S)-1-[[(6-aminohexyl)amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.

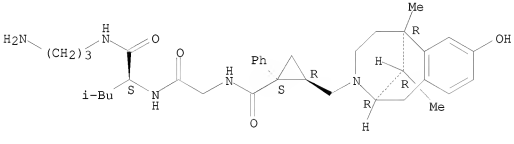


RN 294625-27-7 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-(3-aminopropyl)-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 294624-70-7
CMF C36 H51 N5 O4

Absolute stereochemistry.



CM 2

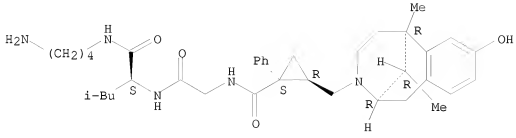
CRN 76-05-1
CMF C2 H F3 O2

RN 294625-28-8 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-(4-aminobutyl)-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 294624-71-8
CMF C37 H53 N5 O4

Absolute stereochemistry.



CM 2

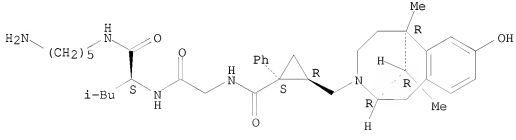
CRN 76-05-1
CMF C2 H F3 O2

RN 294625-29-9 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-(5-aminopentyl)-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 294624-72-9
CMF C38 H55 N5 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

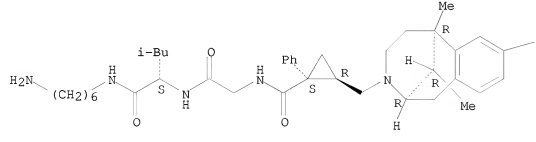
RN 294625-30-2 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-(6-aminohexyl)-, bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 294624-73-0
CMF C39 H57 N5 O4

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

CM 2

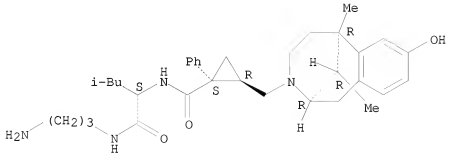
CRN 76-05-1
CMF C2 H F3 O2

RN 294625-31-3 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[(3-aminopropyl)amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 294624-90-1
CMF C34 H48 N4 O3

Absolute stereochemistry.



CM 2

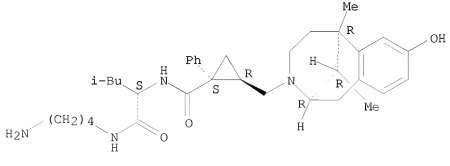
CRN 76-05-1
CMF C2 H F3 O2

RN 294625-32-4 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[(4-aminobutyl)amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 294624-91-2
CMF C35 H50 N4 O3

Absolute stereochemistry.



CM 2

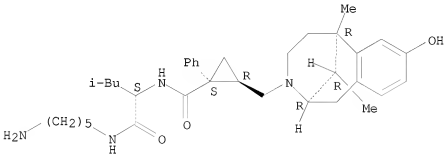
CRN 76-05-1
CMF C2 H F3 O2

RN 294625-33-5 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[(5-aminopentyl)amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 294624-92-3
CMF C36 H52 N4 O3

Absolute stereochemistry.



CM 2

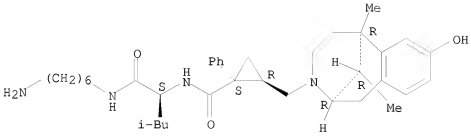
CRN 76-05-1
CMF C2 H F3 O2

RN 294625-34-6 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[(6-aminohexyl)amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 294624-93-4
CMF C37 H54 N4 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 294624-74-1P 294624-75-2P 294624-76-3P
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294624-83-2P 294624-84-3P 294624-85-4P
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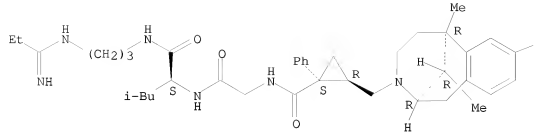
294625-05-1P 294625-06-2P 294625-07-3P
294625-08-4P 294625-09-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and binding affinity of κ-selective agonists)

RN 294624-74-1 CAPLUS

CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[3-[(1-iminopropyl)amino]propyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



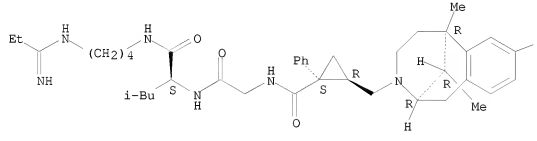
PAGE 1-B

OH

RN 294624-75-2 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[4-[(1-iminopropyl)amino]butyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



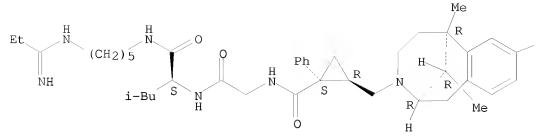
PAGE 1-B

OH

RN 294624-76-3 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[5-[(1-iminopropyl)amino]pentyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

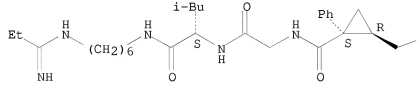


PAGE 1-B

RN 294624-77-4 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[6-[(1-iminopropyl)amino]hexyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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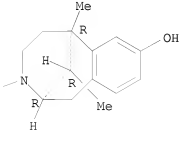
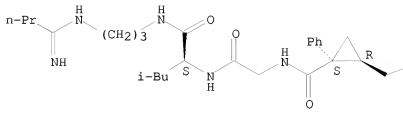


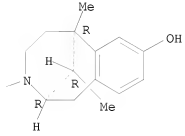
RN 294624-78-5 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[3-[(1-iminobutyl)amino]propyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



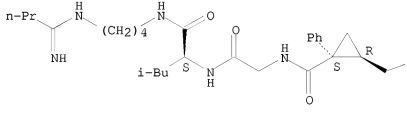
PAGE 1-B



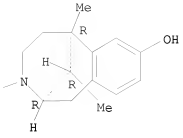
RN 294624-79-6 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[4-[(1-iminobutyl)amino]butyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



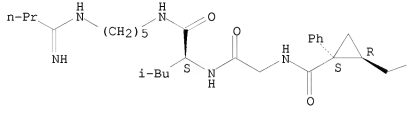
PAGE 1-B



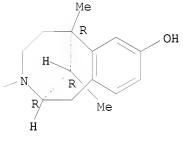
RN 294624-80-9 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[5-[(1-iminobutyl)amino]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



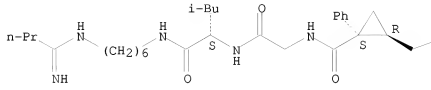
PAGE 1-B



RN 294624-81-0 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[6-[(1-iminobutyl)amino]hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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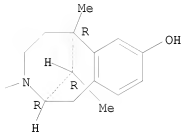
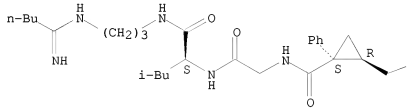


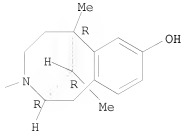
RN 294624-82-1 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[3-[(1-iminopentyl)amino]propyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



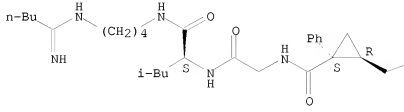
PAGE 1-B



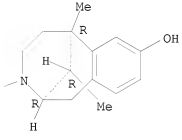
RN 294624-83-2 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[4-[(1-iminopentyl)amino]butyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



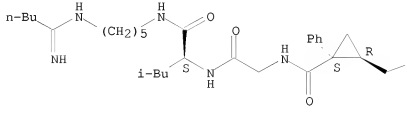
PAGE 1-B



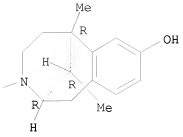
RN 294624-84-3 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[5-[(1-iminopentyl)amino]pentyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



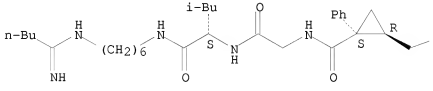
PAGE 1-B



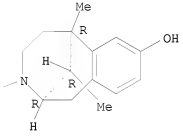
RN 294624-85-4 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[6-[(1-iminopentyl)amino]hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



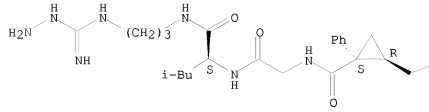
PAGE 1-B



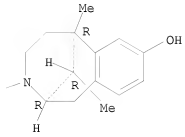
RN 294624-86-5 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[3-[(hydrazinoiminomethyl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



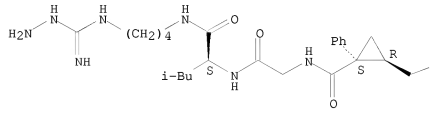
PAGE 1-B



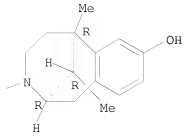
RN 294624-87-6 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[4-[(hydrazinoiminomethyl)amino]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



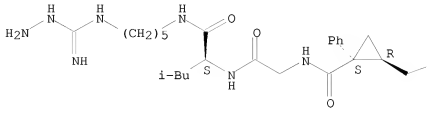
PAGE 1-B



RN 294624-88-7 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[5-[(hydrazinoiminomethyl)amino]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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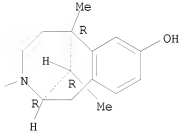

RN 294624-89-8 CAPLUS
CN L-Leucinamide, N-[[(1S,2R)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-N-[6-[(hydrazinoiminomethyl)amino]hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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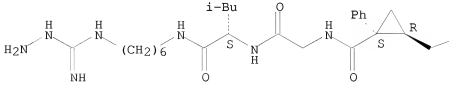
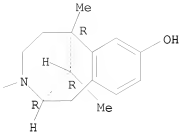
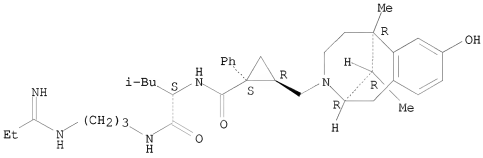




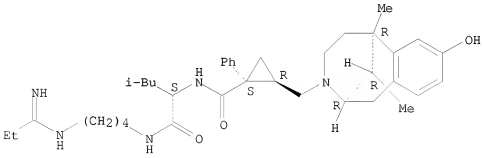
RN 294624-94-5 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[3-[(1-iminopropyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



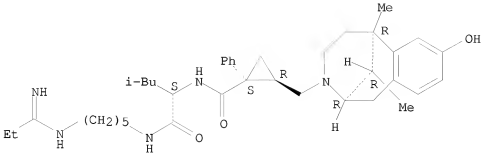
RN 294624-95-6 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[4-[(1-iminopropyl)amino]butyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



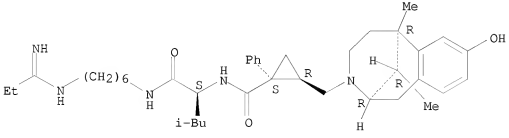
RN 294624-96-7 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[5-[(1-iminopropyl)amino]pentyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



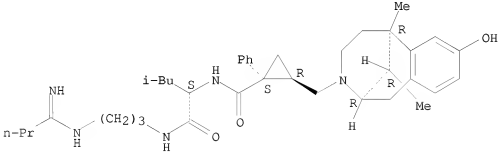
RN 294624-97-8 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[6-[(1-iminopropyl)amino]hexyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



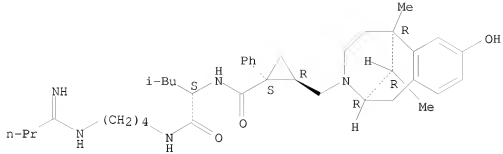
RN 294624-98-9 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[3-[(1-iminobutyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



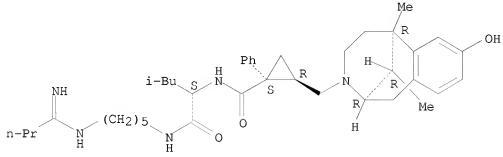
RN 294624-99-0 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[4-[(1-iminobutyl)amino]butyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



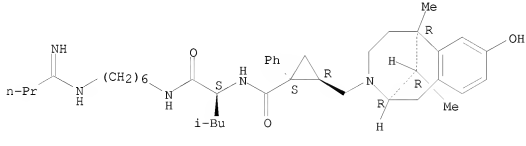
RN 294625-00-6 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[5-[(1-iminobutyl)amino]pentyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



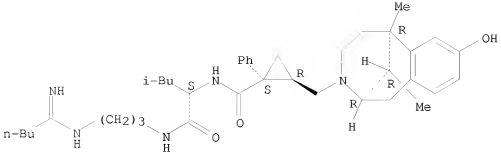
RN 294625-01-7 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[6-[(1-iminobutyl)amino]hexyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



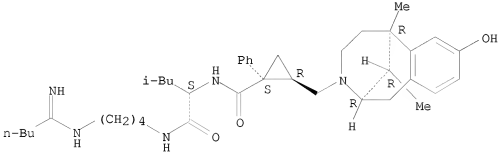
RN 294625-02-8 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[3-[(1-iminopentyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



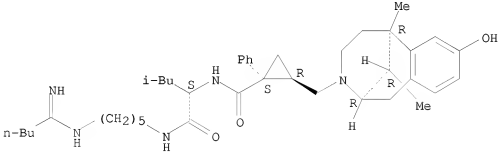
RN 294625-03-9 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[4-[(1-iminopentyl)amino]butyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



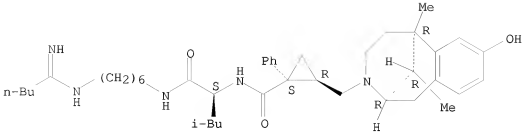
RN 294625-04-0 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[5-[(1-iminopentyl)amino]pentyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



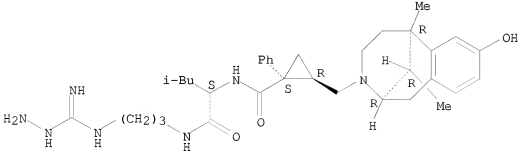
RN 294625-05-1 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[6-[(1-iminopentyl)amino]hexyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



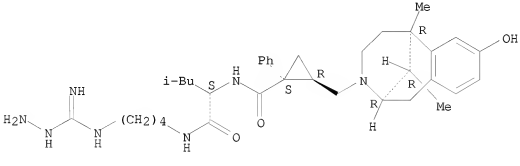
RN 294625-06-2 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[3-[(hydrazinyliminomethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



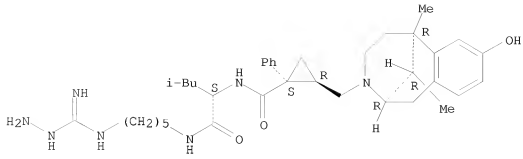
RN 294625-07-3 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[4-[(hydrazinyliminomethyl)amino]butyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



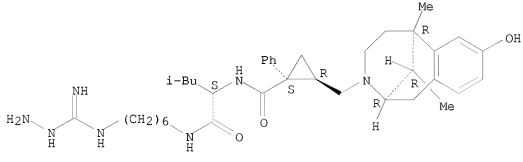
RN 294625-08-4 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[5-[(hydrazinyliminomethyl)amino]pentyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



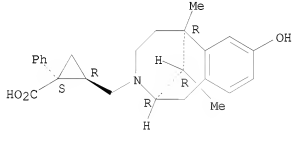
RN 294625-09-5 CAPLUS
CN Cyclopropanecarboxamide, N-[(1S)-1-[[[6-[(hydrazinyliminomethyl)amino]hexyl]amino]carbonyl]-3-methylbutyl]-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 149343-48-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and binding affinity of κ-selective agonists)
RN 149343-48-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
AB A series of 1-phenyl-2-cyclopropylmethylamines structurally related to (+)- and (-)-MPCB were synthesized and their binding affinities for σ1, σ2, opioid and dopamine (D2) receptors were evaluated.

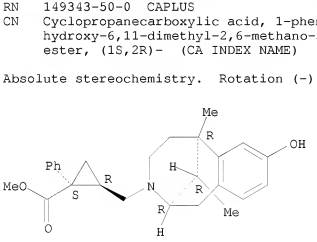
Substitution of the cis-N-normetazocine with different aminic moieties provided compds. with high affinity and selectivity for σ binding sites with respect to opioid and dopamine (D2) receptors. The observed increase in σ2 affinity as compared to the parent (+)-MPCB, supports the idea that the particular stereochem. of (+)-cis-N-normetazocine affects σ1 selectivity but does not affect σ1 affinity. The (±)-cis isomers of Me 2-[(1-adamantylamino)methyl]-1-phenylcyclopropane-1-carboxylate (I) displayed a higher affinity and selectivity for the σ1 and σ2 receptor subtypes compared to the (±)-trans isomers. Interestingly, the enantiomer (-)-cis I displayed a preference for σ1 receptor subtype whereas the (+)-cis I did for σ2. These results prompt the authors to synthesize compds. with modification of nitrogen and carboxyl groups. The compds. obtained showed high affinities and selectivity for σ sites. Moreover, modifications of carboxyl groups provided compds. with the highest affinities in the series. In particular, (±)-cis-{2-[(1-adamantylamino)methyl]-1-phenylcyclopropyl}methyl acetate with reverse-type ester showed a Ki of 0.6 and 4.05 nM for σ1 and σ2 binding sites, resp.

ACCESSION NUMBER: 2000:454843 CAPLUS
DOCUMENT NUMBER: 133:202576
TITLE: Substituted 1-phenyl-2-cyclopropylmethylamines with high affinity and selectivity for sigma sites
AUTHOR(S): Ronsisvalle, G.; Marrazzo, A.; Prezzavento, O.; Pasquinucci, L.; Falcucci, B.; Di Toro, R.; Spampinato, S.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Catania, Catania, 95125, Italy
SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(6), 1503-1513
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

IT 149343-50-0 199999-67-2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(substituted phenylcyclopropylmethylamines with high affinity and selectivity for sigma sites in relation to structure)

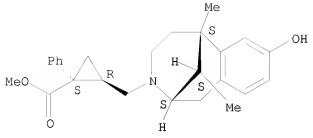
RN 149343-50-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

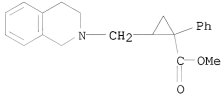


RN 199999-67-2 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 290341-99-0P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(substituted phenylcyclopropylmethylamines with high affinity and selectivity for sigma sites in relation to structure)
RN 290341-99-0 CAPLUS
CN Cyclopropanecarboxylic acid, 2-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]-1-phenyl-, methyl ester (CA INDEX NAME)

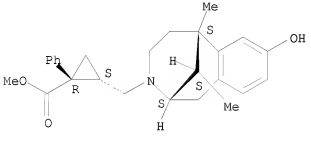


REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
AB The interaction of the κ-opioid receptor with arylacetamide and benzomorphan derivs. acting as agonists was modeled through pharmacophore-based and docking calcns. Potentially bioactive conformations of representative ligands (U-50,488 and its benzo-fused analogs 4 and 6 for arylacetamides and MPCB for benzomorphans) were identified by systematic conformational anal. and docked into a 3D model of the κ-receptor. The obtained complexes, refined by energy-minimization and mol. dynamics, were evaluated for their consistency with structure-activity relationships and site-directed mutagenesis data. The following interactions are hypothesized to govern the ligand-receptor recognition process: (i) a salt bridge between the Asp138 carboxylate and the protonated nitrogen of the bound agonist; (ii) a hydrogen bond donated by the Tyr312 hydroxyl to the carbonyl oxygen of arylacetamides and MPCB; (iii) hydrophobic interactions established by the dichlorophenyl moiety of arylacetamides and the pendant Ph ring of MPCB with the surrounding side chains of Tyr312, Leu224, Leu295, and Ala298; (iv) a π-stacking contact between the Tyr312 side chain and the Ph ring of arylacetamides; (v) a hydrogen bond linking the His291 imidazole ring to the phenolic hydroxy group featured by typical benzomorphans and the arylacetamides 4 and 6.
ACCESSION NUMBER: 2000:316268 CAPLUS
DOCUMENT NUMBER: 133:99072
TITLE: Modeling of κ-opioid receptor/agonists interactions using pharmacophore-based and docking simulations
AUTHOR(S): Lavecchia, Antonio; Greco, Giovanni; Novellino,

Ettore; Vittorio, Franco; Ronsisvalle, Giuseppe
CORPORATE SOURCE: Dipartimento di Chimica Farmaceutica e Tossicologica, Universita di Napoli Federico II, Naples, I-80131, Italy
SOURCE: Journal of Medicinal Chemistry (2000), 43(11), 2124-2134
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 199999-64-9P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(modeling of κ-opioid receptor/agonists interactions using pharmacophore-based and docking simulations)
RN 199999-64-9 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1R,2S)- (CA INDEX NAME)

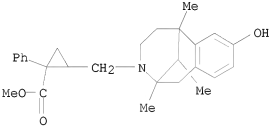
Absolute stereochemistry. Rotation (+).



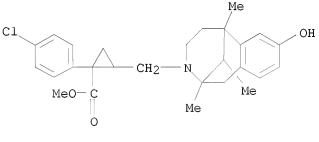
REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
AB Using cyclodextrin capillary zone electrophoresis (CD-CZE), baseline separation of synthetic potential analgesic drug diastereoisomer candidates 6,11-dimethyl-1,2,3,4,5,6-hexahydro-3-[(2'-methoxycarbonyl-2'-phenylcyclopropyl)methyl]-2,6-methano-3-benzazocin-8-ol (MPCB) and 6,11-dimethyl-1,2,3,4,5,6-hexahydro-3-{[2'-methoxycarbonyl-2'(4-chloro phenyl)cyclopropyl]methyl}-2,6-methano-3-benzazocin-8-ol (CCB) was achieved. Among the cyclodextrins tested (hydroxypropyl-, carboxymethyl- and sulfobutyl-β-cyclodextrin (HP-β-CD, CM-β-CD and SBE-β-CD)) SBE-β-CD was found to be the most effective complexing agent, allowing good optical isomer separation Resolution was also influenced by the CD concentration, pH of the buffer and presence of organic modifier in the background electrolyte. The optimum exptl. conditions for the separation of studied analgesic drugs were found using 25 mM borate buffer at pH 9 containing 40 mM of SBE-β-CD and 20% volume/volume of methanol. Using the above-mentioned background electrolyte, it was also possible to sep., in the same run, the enantiomers of normetazocine (NMZ) as well as the optical isomers of (±)-cis-2-chloromethyl-1-Ph cyclopropancarboxylic acid Me ester (PCE) or (±)-cis-2-chloromethyl-1-(4-chlorophenyl)cyclopropancarboxylic acid Me ester (CPCE) reagents used in the synthesis of the studied analgesic drugs.
ACCESSION NUMBER: 1999:623074 CAPLUS
DOCUMENT NUMBER: 131:342123

TITLE: Optical isomer separation of potential analgesic drug candidates by using capillary electrophoresis
AUTHOR(S): Ferrara, Giuseppina; Santagati, Natale Alfredo; Aturki, Zeineb; Fanali, Salvatore
CORPORATE SOURCE: Istituto di Cromatografia del C.N.R., Rome, 00016, Italy
SOURCE: Electrophoresis (1999), 20(12), 2432-2437
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 249934-72-3 249934-73-4
RL: ANT (Analyte); ANST (Analytical study)
(analgesic drug candidates optical isomer separation by capillary electrophoresis using β-cyclodextrin)
RN 249934-72-3 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[(1,4,5,6-tetrahydro-8-hydroxy-2,6,11-trimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester (CA INDEX NAME)



RN 249934-73-4 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(4-chlorophenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-2,6,11-trimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
AB The synthesis and the in vitro receptor affinity for σ1 and opioid receptors of the two diastereoisomers of (+)-cis-MPCB namely, (+)-cis-(1'S,2'R)-6,11-Dimethyl-1,2,3,4,5,6-hexahydro-3-[[2'-(methoxycarbonyl)-2'-phenylcyclopropyl]methyl]-2,6-methano-3-benzazocin-8-ol, (1'S,2'R)6a and (+)-cis-(1'R,2'S)-6,11-Dimethyl-1,2,3,4,5,6-hexahydro-3-[[2'-(methoxycarbonyl)-2'-phenylcyclopropyl]methyl]-2,6-methano-3-benzazocin-8-ol, (1'R,2'S)6a are reported. Affinities of (1'S,2'R)6a and (1'R,2'S)6a were compared with those of the (-)-cis-diastereoisomers of MPCB(1), and of its p-Cl Ph derivative CCB(2). The (+)-cis-N-normetazocine

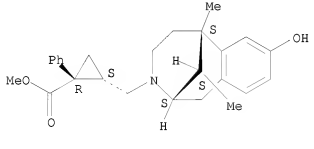
derivs. showed higher affinity for the σ1 sites, labeled with [3H]-(+)-pentazocine than the corresponding (-)-cis- analogs. In particular, compound (1'S,2'R)6a showed a Ki = 66.7 nM for σ1 receptor, associated with a good selectivity for σ1 with respect to κ, μ, δ opioid receptors subtypes (Ki = > 1,000 nM). Anal. of the data seem to support the hypothesis that the (+)-cis-N-normetazocine nucleus possess a specific enantioselectivity for σ1 sites, when supporting bulkier N-substituents functionalized with a carboxy ester group.

ACCESSION NUMBER: 1997:698529 CAPLUS
DOCUMENT NUMBER: 128:43727
ORIGINAL REFERENCE NO.: 128:8431a,8434a
TITLE: Synthesis of (+)-(1'R,2'S) and (1'S,2'R)-6,11-dimethyl-1,2,3,4,5,6-hexahydro-3-[[2'-(alkoxycarbonyl)-2'-phenylcyclopropyl]methyl]-2,6-methano-3-benzazocin-8-ol. Comparison of the affinities for σ1 and opioid receptors with in the diastereoisomeric MPCB and CCB
AUTHOR(S): Ronsisvalle, Giuseppe; Prezzavento, Orazio; Pasquinucci, Lorella; Pappalardo, Maria S.; Marrazzo, Agostino; Vittorio, Franco; Carboni, Lucia; Spampinato, Santi
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita di Catania, Catania, 95125, Italy
SOURCE: Farmaco (1997), 52(6-7), 471-476
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Societa Chimica Italiana
DOCUMENT TYPE: Journal
LANGUAGE: English

IT 199999-64-9P 199999-67-2P 199999-69-4P
199999-71-8P 199999-73-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and opioid receptor binding by (+)-cis-MPCB diastereomers)

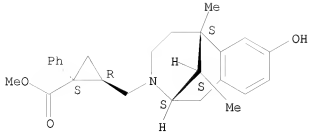
RN 199999-64-9 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



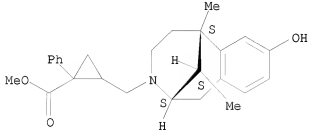
RN 199999-67-2 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



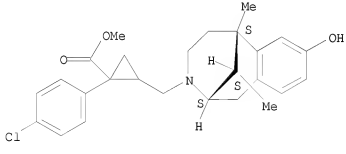
RN 199999-69-4 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



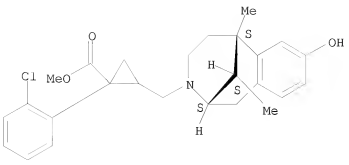
RN 199999-71-8 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(4-chlorophenyl)-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 199999-73-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(2-chlorophenyl)-2-[[(2S,6S,11S)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



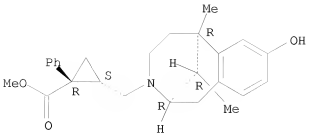
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

AB In previous studies, MPCB and CCB were proposed as possible peptidomimetics of the N-terminal peptide fragment of κ-selective endogenous ligands, such as dynorphin A. With the aim of supporting this hypothesis and assessing the contribution given by the C-terminal residue in receptor interaction, the authors synthesized hybrid ligands linking selected peptide fragments and evaluated their binding affinity of both native and cloned κ-opioid receptors expressed in CHO-K1 cells, using [3H]U69,593 as labeled ligand. All the compds. showed an affinity for κ receptors significantly higher than that of MPCB and, in particular, MPCB-RRI bound to the cloned κ receptor with a Ki value in the low nanomolar range. These results seem to confirm the role of κ pharmacophore played by MPCB and CCB, which are able to activate selectively κ receptors and are suitable supports for basic amino acid residues, critical for the recognition of accessory receptor sites.

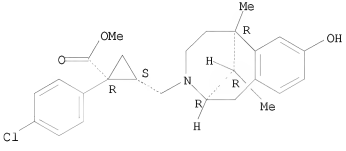
ACCESSION NUMBER: 1997:348655 CAPLUS
DOCUMENT NUMBER: 127:45095
ORIGINAL REFERENCE NO.: 127:8455a,8458a
TITLE: Peptidomimetics of the κ-opioid receptor. A hybrid MPCB/peptide ligand (MPCB-RRI) binds κ cloned receptor with nanomolar affinity
AUTHOR(S): Ronsisvalle, G.; Pappalardo, M. S.; Carboni, L.; Vittorio, F.; Pasquinucci, L.; Marrazzo, A.; Cacciaguerra, S.; Spampinato, S.
CORPORATE SOURCE: Institute of Pharmaceutical Chemistry, University of Catania, Catania, 95125, Italy
SOURCE: Analgesia (Elmsford, New York) (1996), 2(5/6), 283-286
CODEN: AALGEB; ISSN: 1071-569X
PUBLISHER: Cognizant Communication Corp.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 149343-51-1 154711-57-6 191024-90-5 191024-92-7 191024-94-9 191024-96-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(peptidomimetics hybrids of MPCB/peptide type binds κ-opioid receptor with nanomolar affinity)
RN 149343-51-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



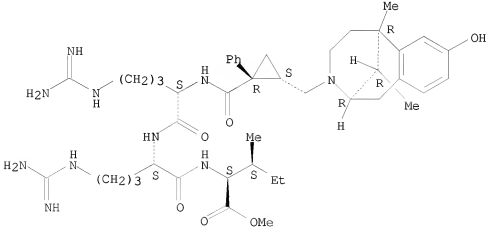
RN 154711-57-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(4-chlorophenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2R-[2α,3(1R*,2S*),6α,11R*]]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 191024-90-5 CAPLUS
CN L-Isoleucine, N2-[[(1R,2S)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]-L-arginyl-L-arginyl-, methyl ester (CA INDEX NAME)

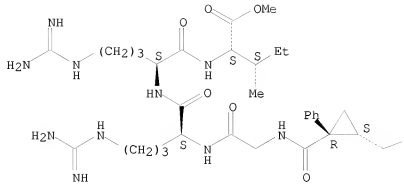
Absolute stereochemistry.



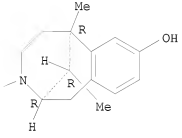
RN 191024-92-7 CAPLUS
CN L-Isoleucine, N-[[(1R,2S)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]glycyl-L-arginyl-L-arginyl-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



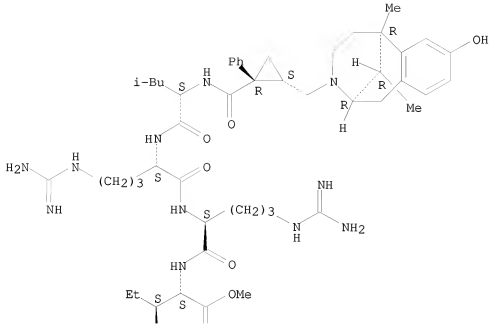
PAGE 1-B



RN 191024-94-9 CAPLUS
CN L-Isoleucine, N-[[(1R,2S)-1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]-L-leucyl-L-arginyl-L-arginyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

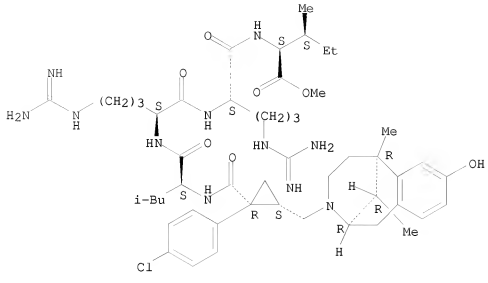
PAGE 1-A



PAGE 2-A

RN 191024-96-1 CAPLUS
CN L-Isoleucine, N-[[(1R,2S)-1-(4-chlorophenyl)-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]cyclopropyl]carbonyl]-L-leucyl-L-arginyl-L-arginyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

AB CCB, 6,11-dimethyl-1,2,3,4,5,6-hexahydro-3-{[2'-methoxycarbonyl-2'-(4-chlorophenyl)cyclopropyl]methyl}-2,6-methano-3-benzazocin-8-ol, displays specificity and very high affinity for κ opioid receptor types (Ki = 0.41 nM). In contrast to other κ opioid agonists, CCB is also selective with respect to σ1 sites (Ki = 1,050 nM). CCB displays antinociceptive and sedative effects in the mouse comparable to those of U50,488H and morphine. Naltrexone fully antagonizes these effects. The sedative effects of CCB are blocked in mice pretreated with naltrexone or nor-BNI. CCB and U50,488H produce a superimposable diuresis in rats. Naltrexone and nor-BNI, both are effective in antagonizing the effect. CCB does not produce any stereotyped behavior or ataxia in the behavioral assay in doses up to 40 mg/kg, s.c. These findings suggest that CCB might be a useful tool to investigate the physiol. role of κ opioid receptors.

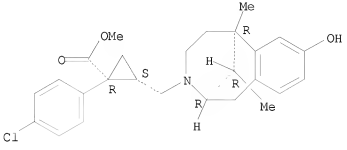
ACCESSION NUMBER: 1995:807823 CAPLUS
DOCUMENT NUMBER: 123:247166
ORIGINAL REFERENCE NO.: 123:43915a,43918a
TITLE: CCB, a novel specific κ opioid agonist, which discriminates between opioid and σ1 recognition sites
AUTHOR(S): Ronsisvalle, G.; Prezzavento, O.; Pasquinucci, L.; Marrazzo, A.; Vittorio, F.; Gomez-Vidal, J. A.; Carboni, L.; Spampinato, S.
CORPORATE SOURCE: Institute Pharmaceutical Chemistry, University Catania, Catania, Italy
SOURCE: Life Sciences (1995), 57(16), 1487-95
CODEN: LIFSAK; ISSN: 0024-3205
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

IT 154711-57-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(benzomorphan derivative as κ opioid agonist discriminating between opioid and σ1 recognition sites)

RN 154711-57-6 CAPLUS

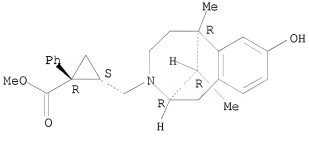
CN Cyclopropanecarboxylic acid, 1-(4-chlorophenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2R-[2α,3(1R*,2S*),6α,11R*]]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



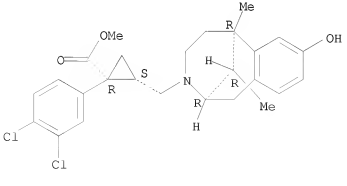
IT 149343-51-1 154711-58-7 155566-31-7
168102-68-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(opioid receptor binding affinity of benzomorphan derivs.)
RN 149343-51-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



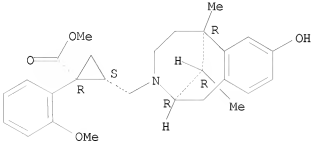
RN 154711-58-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(3,4-dichlorophenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2R-[2α,3(1R*,2S*),6α,11R*]]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

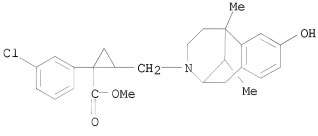


RN 155566-31-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(2-methoxyphenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2α,3(1R*,2S*),6α,11R*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Currently available stereo shown.



RN 168102-68-9 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(3-chlorophenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2S-[2α,3(1S*,2S*),6α,11R*]]- (9CI) (CA INDEX NAME)



L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
AB CCB, a chloro substituted derivative of MPCB, a recently synthesized kappa specific opioid agonist, has been shown to maintain specificity for the kappa receptor associated with a binding affinity 2.6 times higher than that of U50488H. Structure-activity relationships are discussed for (1'R,2'S)/(1'S,2'R)-6-11dimethyl-1,2,3,4,5,6-hexahydro-3[(2'-(methoxycarbonyl)-2(4''-chlorophenylcyclopropyl)]methyl]2,6-methano-3-benzazocin-8-ol (MPCB) and U50488H analogs.

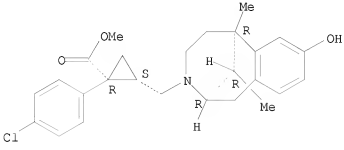
ACCESSION NUMBER: 1994:400235 CAPLUS
DOCUMENT NUMBER: 121:235
ORIGINAL REFERENCE NO.: 121:39a,42a
TITLE: CCB: a novel analog of MPCB with high binding affinity and specific kappa opioid receptor agonist
AUTHOR(S): Ronsisvalle, G.; Prezzavento, O.; Pasquinucci, L.; Carboni, L.; Pistacchio, E.; Spampinato, S.
CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Catania, Catania, 95125, Italy
SOURCE: Regulatory Peptides (1994), (Suppl. 1), S31-S32
CODEN: REPPDY; ISSN: 0167-0115
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 154711-57-6 154711-58-7 154801-95-3 155566-19-1, PMCB 155566-31-7, OMCB

RL: BIOL (Biological study)
(κ-opioid receptor binding and analgesic activity of, structure in relation to)

RN 154711-57-6 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(4-chlorophenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2R-[2α,3(1R*,2S*),6α,11R*]]- (9CI) (CA INDEX NAME)

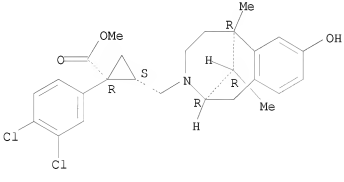
Relative stereochemistry.



RN 154711-58-7 CAPLUS

CN Cyclopropanecarboxylic acid, 1-(3,4-dichlorophenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2R-[2α,3(1R*,2S*),6α,11R*]]- (9CI) (CA INDEX NAME)

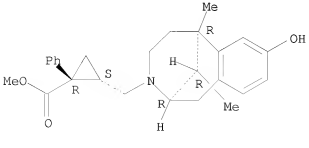
Relative stereochemistry.



RN 154801-95-3 CAPLUS

CN Cyclopropanecarboxylic acid, 1-phenyl-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2α,3(1R*,2S*),6α,11R*]- (9CI) (CA INDEX NAME)

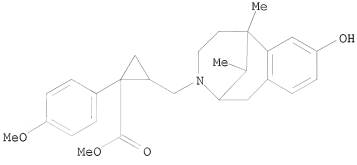
Relative stereochemistry.



RN 155566-19-1 CAPLUS

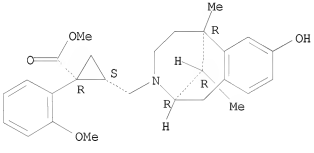
CN Cyclopropanecarboxylic acid, 1-(4-methoxyphenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2α,3(1R*,2S*),6α,11R*]- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 155566-31-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-(2-methoxyphenyl)-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2α,3(1R*,2S*),6α,11R*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Currently available stereo shown.



L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
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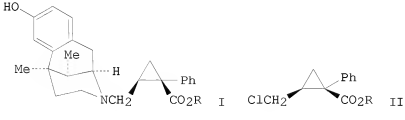


AB A series of Ph carboxy esters I (R = Me, Et, Pr, Bu) derived from normetazocine was synthesized and evaluated for its selectivity at μ, κ, and δ opioid receptors. Compound I (R = Me), although 43 times less potent than the reference compound U50488, was specific for κ receptors, having no detectable affinity for either μ or δ

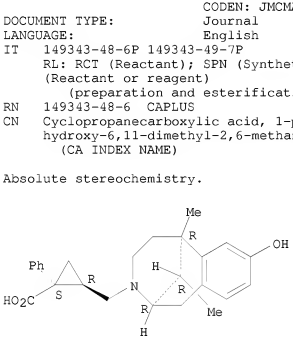
receptors. Greater binding affinity was seen with the diastereoisomer having the 1'R,2'S stereochem. in the cyclopropyl ring of the nitrogen substituent, which was only 12 times less active than U50488. Antinociceptive activity in the mouse tail flick was only slightly lower than that of U50488 (ED50 = 7.66 vs 4.52 mg/kg). Naloxone fully prevented antinociception induced by (1'R,2'S)-I (R = Me) at the doses of 2.0 mg/kg. Compound (1'R,2'S)-I (R = Me) is one of the most κ-selective non-peptide compds. reported to date. The implications of these results in terms of requirements for κ ligands are discussed.

ACCESSION NUMBER: 1993:517591 CAPLUS
DOCUMENT NUMBER: 119:117591
ORIGINAL REFERENCE NO.: 119:21171a,21174a
TITLE: Non-peptide ligands for opioid receptors. Design of κ-specific agonists
AUTHOR(S): Ronsisvalle, G.; Pasquinucci, L.; Pappalardo, M. S.; Vittorio, F.; Fronza, G.; Romagnoli, C.; Pistacchio, E.; Spampinato, S.; Ferri, S.
CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Catania, Catania, 95125, Italy
SOURCE: Journal of Medicinal Chemistry (1993), 36(13), 1860-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

IT 149343-48-6P 149343-49-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)

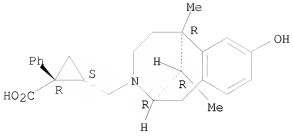
RN 149343-48-6 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1S,2R)-
(CA INDEX NAME)

Absolute stereochemistry.

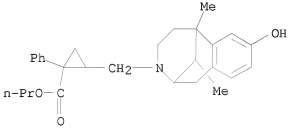


RN 149343-49-7 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1R,2S)-
(CA INDEX NAME)

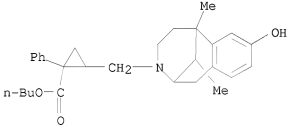
Absolute stereochemistry.



IT 149270-46-2P 149270-47-3P 149343-50-0P
149343-51-1P 154801-95-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and opioid receptor binding affinity of)
RN 149270-46-2 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, propyl ester, [2α,3(1R*,2S*),6α,11R*]- (9CI) (CA INDEX NAME)

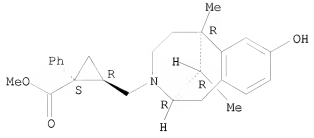


RN 149270-47-3 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, butyl ester, [2α,3(1R*,2S*),6α,11R*]- (9CI) (CA INDEX NAME)



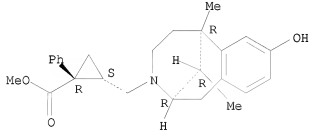
RN 149343-50-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



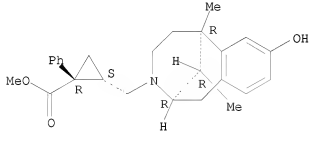
RN 149343-51-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, methyl ester, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

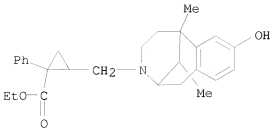


RN 154801-95-3 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, methyl ester, [2α,3(1R*,2S*),6α,11R*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

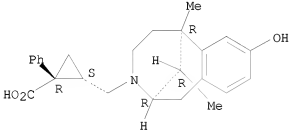


IT 149270-45-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, ester hydrolysis, and opioid receptor binding affinity of)
RN 149270-45-1 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[(1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl)methyl]-, ethyl ester, [2α,3(1R*,2S*),6α,11R*]- (9CI) (CA INDEX NAME)



IT 149270-52-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, resolution, and opioid receptor binding affinity of)
RN 149270-52-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-phenyl-2-[[(2R,6R,11R)-1,4,5,6-tetrahydro-8-hydroxy-6,11-dimethyl-2,6-methano-3-benzazocin-3(2H)-yl]methyl]-, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
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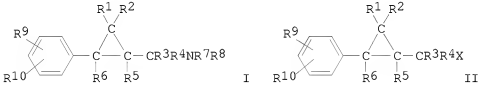


AB The title compds. I (R1-6 = H, C1-4 alkyl, halo; R7, R8 = H, C1-4 alkyl; or NR7R8 = heterocyclic ring optionally containing addnl. hetero atom; R9, R10 = H, halo, alkyl, alkenyl, aryl, cycloalkyl, alkoxy, aryloxy, trihydrocarbylsilyl, etc.), useful as fungicides, are prepared (174 compds.). Thus, for example, 0.53 g II (R1-6 = R9 = H, X = Cl, R10 = p-Me3C) and 1 mL piperidine were heated at 80° for 10 h in pyridine to give 0.3 g I (R1-6 = R9 = H, NR7R8 = piperidino, R10 = p-Me3C) (III), which at 0.05% was 100% effective in controlling Puccinia recondita on wheat. Formulations are also described, e.g. a seed dressing containing II 50, mineral oil 2, and china clay 48%.

ACCESSION NUMBER: 1986:626008 CAPLUS
DOCUMENT NUMBER: 105:226008
ORIGINAL REFERENCE NO.: 105:36479a,36482a
TITLE: Phenylcyclopropylalkylamines
INVENTOR(S): Worthington, Paul Anthony; Sugavanam, Balasubramanyan

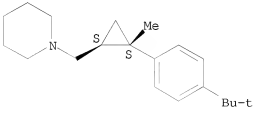
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK
SOURCE: Eur. Pat. Appl., 101 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 188887	A1	19860730	EP 1985-309054	19851212	<--
EP 188887	B1	19910502			
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE					
GB 2170197	A	19860730	GB 1985-30644	19851212	<--
GB 2170197	B	19880824			
AT 63113	T	19910515	AT 1985-309054	19851212	<--
AU 8551389	A	19860724	AU 1985-51389	19851218	<--
ZA 8600047	A	19860827	ZA 1986-47	19860103	<--
DK 8600125	A	19860718	DK 1986-125	19860110	<--
BR 8600138	A	19860923	BR 1986-138	19860115	<--
HU 39956	A2	19861128	HU 1986-195	19860115	<--
CN 86100254	A	19861008	CN 1986-100254	19860116	<--
JP 61167648	A	19860729	JP 1986-6588	19860117	<--
ES 550992	A5	19881116	ES 1986-550992	19860117	<--

PRIORITY APPLN. INFO.:			
	GB 1985-1169	A	19850117
	GB 1985-12400	A	19850516
	GB 1985-16804	A	19850703
	GB 1985-20592	A	19850816
	GB 1985-29482	A	19851129
	EP 1985-309054	A	19851212

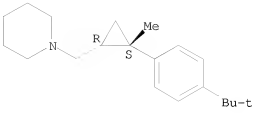
OTHER SOURCE(S): CASREACT 105:226008; MARPAT 105:226008
IT 105358-42-7P 105358-43-8P 105392-87-8P
105392-91-4P 105393-05-3P 105393-59-7P
105455-08-1P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as fungicide)
RN 105358-42-7 CAPLUS
CN Piperidine, 1-[[2-[4-(1,1-dimethylethyl)phenyl]-2-methylcyclopropyl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



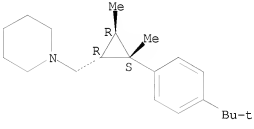
RN 105358-43-8 CAPLUS
CN Piperidine, 1-[[2-[4-(1,1-dimethylethyl)phenyl]-2-methylcyclopropyl]methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



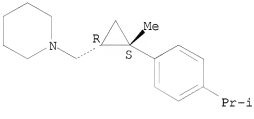
RN 105392-87-8 CAPLUS
CN Piperidine, 1-[[2-[4-(1,1-dimethylethyl)phenyl]-2,3-dimethylcyclopropyl]methyl]-, (1α,2α,3β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



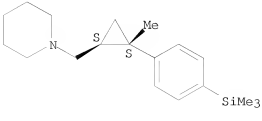
RN 105392-91-4 CAPLUS
CN Piperidine, 1-[[2-methyl-2-[4-(1-methylethyl)phenyl]cyclopropyl]methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 105393-05-3 CAPLUS
CN Piperidine, 1-[[2-methyl-2-[4-(trimethylsilyl)phenyl]cyclopropyl]methyl]-, trans- (9CI) (CA INDEX NAME)

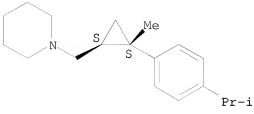
Relative stereochemistry.



RN 105393-59-7 CAPLUS

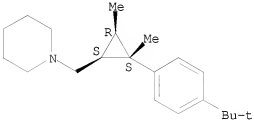
CN Piperidine, 1-[[2-methyl-2-[4-(1-methylethyl)phenyl]cyclopropyl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

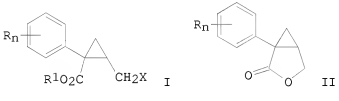


RN 105455-08-1 CAPLUS
CN Piperidine, 1-[[2-[4-(1,1-dimethylethyl)phenyl]-2,3-dimethylcyclopropyl]methyl]-, (1α,2β,3α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
GI



AB Title esters I (R = H, halo, C1-C4 alkyl or alkoxy, NO2, NH2, SO2NH2, OH; n = 1-3; Rn may be benzo; R1 = C1-C5 alkyl or alkenyl, aryl, PhCH2; X = NR2R3; R2, R3 = H, C1-C5 alkyl, alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, carboxyalkyl, dialkylaminoalkyl, aryl, arylalkyl, cycloalkyl; R2R3N = 5- or 6-membered heterocyclyl) were prepared by cleaving lactones II with R1OH and a thionyl halide, followed by amination of I (X = halo). Thus, SOCl2 and then II (Rn = H) were added, with stirring, to EtOH at -10° and the mixture kept 12 h at room temperature to give 95% I (Rn = H, R1 = Et, X = Cl), which were aminated with various amines in refluxing PhMe.

ACCESSION NUMBER: 1983:178811 CAPLUS
DOCUMENT NUMBER: 98:178811
ORIGINAL REFERENCE NO.: 98:27163a,27166a
TITLE: (Z)-1-Aryl-2-(aminomethyl)cyclopropanecarboxylates and their use as medicines in the treatment of various

disorders

INVENTOR(S): Cousse, Henri; Mouzin, Gilbert; Bonnaud, Bernard; Charveron, Marie; Fauran, Francois

PATENT ASSIGNEE(S): Fabre, Pierre, S. A., Fr.

SOURCE: Eur. Pat. Appl., 61 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 68998	A1	19830105	EP 1982-401128	19820621	<--
EP 68998	B1	19850828			
R: AT, BE, CH, DE, GB, IT, LI, LU, NL, SE					
FR 2508033	A1	19821224	FR 1981-12311	19810623	<--
FR 2508033	B1	19840629			
AT 15181	T	19850915	AT 1982-401128	19820621	<--
CA 1199929	A1	19860128	CA 1982-405587	19820621	<--
AU 8285087	A	19830106	AU 1982-85087	19820622	<--
AU 553924	B2	19860731			
JP 58000945	A	19830106	JP 1982-107520	19820622	<--
ZA 8204403	A	19830427	ZA 1982-4403	19820622	<--
US 4507318	A	19850326	US 1982-390811	19820622	<--
US 4567288	A	19860128	US 1984-656443	19841001	<--

PRIORITY APPLN. INFO.:	FR 1981-12311	A	19810623
	EP 1982-401128	A	19820621
	US 1982-390811	A1	19820622

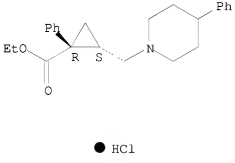
OTHER SOURCE(S): CASREACT 98:178811; MARPAT 98:178811

IT 85467-42-1P 85467-45-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 85467-42-1 CAPLUS

CN Cyclopropanecarboxylic acid, 1-phenyl-2-[(4-phenyl-1-piperidinyl)methyl]-, ethyl ester, hydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

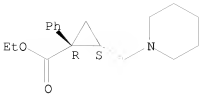


● HCl

RN 85467-45-4 CAPLUS

CN Cyclopropanecarboxylic acid, 1-phenyl-2-(1-piperidinylmethyl)-, ethyl ester, hydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

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CA SUBSCRIBER PRICE                                     -12.30     -12.30

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STRUCTURE FILE UPDATES:   18 MAY 2009  HIGHEST RN 1147182-17-9
DICTIONARY FILE UPDATES:  18 MAY 2009  HIGHEST RN 1147182-17-9

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

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predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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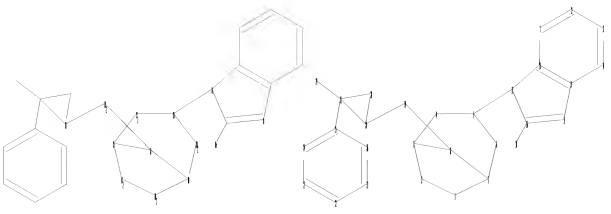

chain nodes :
18 19 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 20 21 22 23 24 25
26 27 28
chain bonds :
5-17 8-19 16-18 19-20 21-25 21-29
ring bonds :
1-2 1-7 2-3 3-4 3-8 4-5 5-6 6-7 7-8 9-10 9-14 9-15 10-11 10-17 11-12
12-13 13-14 15-16 16-17 20-21 20-28 21-28 22-23 22-27 23-24 24-25 25-26
26-27
exact/norm bonds :
1-2 1-7 2-3 3-4 3-8 4-5 5-6 5-17 6-7 7-8 9-15 10-17 15-16 16-17 20-21
20-28 21-28
exact bonds :
8-19 16-18 19-20 21-25 21-29
normalized bonds :
9-10 9-14 10-11 11-12 12-13 13-14 22-23 22-27 23-24 24-25 25-26 26-27

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom
29:CLASS

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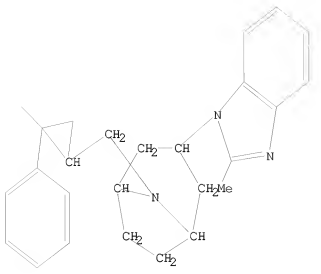
L5 STR



Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 119 TO ITERATE

100.0% PROCESSED 119 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

L6 8 SEA SSS FUL L5

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	186.36	472.78
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CA SUBSCRIBER PRICE	0.00	-12.30

FILE 'CAPLUS' ENTERED AT 11:08:12 ON 20 MAY 2009
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FILE COVERS 1907 - 20 May 2009 VOL 150 ISS 21
FILE LAST UPDATED: 19 May 2009 (20090519/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate

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L7 1 L6

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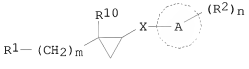
L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN
GI



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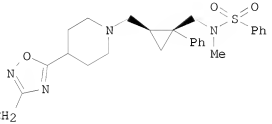

II

AB Title compds. I [R1 = (un)substituted saturated, partially saturated, or aromatic 4-7 monocyclic or 8-10 membered bicyclic ring having one ring nitrogen and 0-4 addnl. heteroatoms selected from O, P, S or N, optionally attached through alkylene chain, substituted-amine, -amide, etc.; R2 = OH, halogen (un)substituted-alkyl, -alkoxy, -aryl, -heteroaryl, -cycloalkyl, etc., optionally two adjacent R2s taken together form a fused, saturated, partially saturated or aromatic 5-6 membered ring having 0-3 heteroatoms selected from O, P, S, or N, or two geminal R2s optionally taken together from a spiro, saturated, partially saturated or aromatic 5-6 membered ring having 0-3 heteroatoms selected from O, P, S or N, said fused or spiro ring being optionally substituted; R10 = H, (un)substituted-alkyl, -alkenyl, -alkynyl, -cycloalkyl, -heterocyclyl, -heteroaryl, or aryl; X = (un)substituted-alkylene chain which optionally may have 0-3 heteroatoms selected from O, P, S or N; A = saturated, partially saturated, or aromatic 3-7 monocyclic or 8-10 membered bicyclic ring having one ring nitrogen and 0-4 addnl. heteroatoms selected from O, P, S or N ; m = 0-3, n = 0-5] and

their pharmaceutically acceptable salts are prepared and disclosed as CCR5 antagonists. Thus, II was prepared by reaction of N-{[(1S,2R)-2-formyl-1-phenylcyclopropyl]methyl}-N-methylbenzenesulfonamide (preparation given) and 4-(3-benzyl-1,2,4-oxadiazol-5-yl)piperidine. Addnl. preparative examples utilizing combinatorial methods of synthesis are given. I have pIC50 values of ≥5 in assays for CCR5 antagonism. As CCR5 antagonists, I are useful for the treatment of viral infections (particularly HIV infection).

ACCESSION NUMBER: 2004:534198 CAPLUS
DOCUMENT NUMBER: 141:88871
TITLE: Preparation of aminoalkylaryl cyclopropyl compounds as CCR5 antagonists
INVENTOR(S): Peckham, Jennifer Poole; Aquino, Christopher Joseph; Kazmierski, Wieslaw Mieczyslaw
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004055010	A2	20040701	WO 2003-US39619	20031212
WO 2004055010	A3	20041223		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003296993	A1	20040709	AU 2003-296993	20031212
EP 1569934	A2	20050907	EP 2003-813416	20031212
EP 1569934	B1	20080123		
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JP 2006514950	T	20060518	JP 2004-560831	20031212
AT 384724	T	20080215	AT 2003-813416	20031212
ES 2298627	T3	20080516	ES 2003-813416	20031212
US 20060052408	A1	20060309	US 2005-538196	20050609

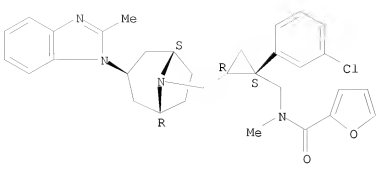
PRIORITY APPLN. INFO.: US 2002-433626P P 20021213
WO 2003-US39619 W 20031212

OTHER SOURCE(S): MARPAT 141:88871

IT 714976-75-7P 714976-77-9P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(preparation of aminoalkylaryl cyclopropane derivs. as CCR5 antagonists)

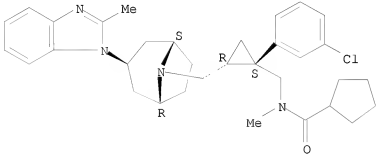
RN 714976-75-7 CAPLUS
CN 2-Furancarboxamide, N-[[(1S,2R)-1-(3-chlorophenyl)-2-[[(3-exo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclopropyl]methyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



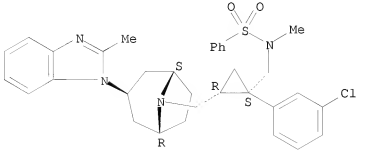
RN 714976-77-9 CAPLUS
CN Cyclopentanecarboxamide, N-[[(1S,2R)-1-(3-chlorophenyl)-2-[[(3-exo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclopropyl]methyl]-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



IT 714976-73-5P 714976-86-0P 714976-87-1P
714976-88-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminoalkylaryl cyclopropane derivs. as CCR5 antagonists)
RN 714976-73-5 CAPLUS
CN Benzenesulfonamide, N-[[(1S,2R)-1-(3-chlorophenyl)-2-[[(3-exo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclopropyl]methyl]-N-methyl- (CA INDEX NAME)

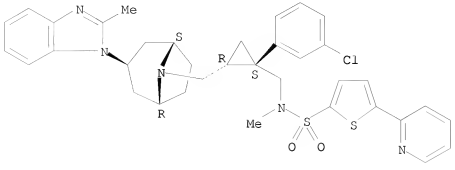
Absolute stereochemistry.



RN 714976-86-0 CAPLUS
CN 2-Thiophenesulfonamide, N-[[(1S,2R)-1-(3-chlorophenyl)-2-[[(3-exo)-3-(2-

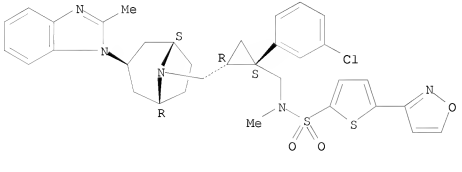
methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclopropyl]methyl]-N-methyl-5-(2-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry.



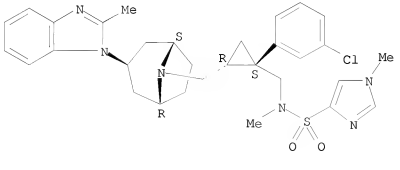
RN 714976-87-1 CAPLUS
CN 2-Thiophenesulfonamide, N-[[(1S,2R)-1-(3-chlorophenyl)-2-[[(3-exo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclopropyl]methyl]-5-(3-isoxazolyl)-N-methyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 714976-88-2 CAPLUS
CN 1H-Imidazole-4-sulfonamide, N-[[(1S,2R)-1-(3-chlorophenyl)-2-[[(3-exo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclopropyl]methyl]-N,1-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.



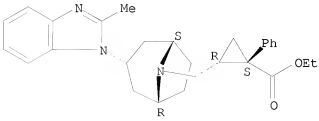
IT 714977-69-2P 714977-70-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminoalkylaryl cyclopropane derivs. as CCR5 antagonists)

RN 714977-69-2 CAPLUS

CN Cyclopropanecarboxylic acid, 2-[[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]-1-phenyl-, ethyl ester, (1S,2R)-(CA INDEX NAME)

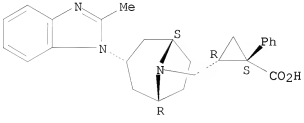
Absolute stereochemistry.



RN 714977-70-5 CAPLUS

CN Cyclopropanecarboxylic acid, 2-[[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]-1-phenyl-, (1S,2R)- (CA INDEX NAME)

Absolute stereochemistry.



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ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y
STN INTERNATIONAL LOGOFF AT 11:09:25 ON 20 MAY 2009